1-(2,4,5-Trimethoxyphenyl)butan-1-one

Inchi: InChI=1S/C13H18O4/c1-5-6-10(14)9-7-12(16-3)13(17-4)8-11(9)15-2/h7-8H,5-6H2,1-4H3
InchiKey: CSBSTMGRAOUNFM-UHFFFAOYSA-N
Formula: C13H18O4
SMILES: CCCC(=O)c1cc(OC)c(OC)cc1OC
Mol. weight [g/mol]: 238.28
CAS: 2020-73-7

Physical Properties

Property code	Value	Unit	Source
gf	-301.82	kJ/mol	Joback Method
hf	-618.77	kJ/mol	Joback Method
hfus	27.46	kJ/mol	Joback Method
hvap	62.77	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.695		Crippen Method
mcvol	189.450	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1891.00		NIST Webbook
rinpol	1891.00		NIST Webbook
tb	659.59	K	Joback Method
tc	861.54	K	Joback Method
tf	416.87	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.68	J/mol×K	659.59	Joback Method
cpg	509.36	J/mol×K	693.25	Joback Method
cpg	523.31	J/mol×K	726.91	Joback Method
cpg	536.50	J/mol×K	760.56	Joback Method
cpg	548.92	J/mol×K	794.22	Joback Method
cpg	560.54	J/mol×K	827.88	Joback Method
cpg	571.35	J/mol×K	861.54	Joback Method

dvisc	0.0006082	Pa×s	416.87	Joback Method
dvisc	0.0003956	Pa×s	457.32	Joback Method
dvisc	0.0002760	Pa×s	497.78	Joback Method
dvisc	0.0002032	Pa×s	538.23	Joback Method
dvisc	0.0001562	Pa×s	578.68	Joback Method
dvisc	0.0001242	Pa×s	619.14	Joback Method
dvisc	0.0001016	Pa×s	659.59	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2020737&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume